Reaction c1OH

k(300)	A	Ea	Notes	
6.62e-15	2.15e-12	3.45	31	CH4 + HO. = H2O + C-O2.

Notes

31	Rate constant expression recommended by IUPAC, Supplement VII (Atkinson et al, 1999).

The reactants, products and rate parameter are consistent with current knowledge.

Reaction ISOH

k(300)	A	Ea	Notes	
9.73e-11	2.50e-11	-0.81	131, 132	ISOPRENE + HO. = #.909 RO2-R. + #.091 RO2-N. + #.079 R2O2. + #.626 HCHO + #.23 METHACRO + #.32 MVK + #.359 ISOPROD + #-.167 XC

Notes

131	Isoprene mechanism used is based on the "four product" condensed isoprene mechanism of Carter (1996) which in turn is based on the detailed isoprene mechanism of Carter and Atkinson (1996). The rate constants and the major initial reaction pathways are the same as used in those mechanisms. Some minor changes in product yields resulted in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction schemes, or as indicated in other footnotes.
132	The overall nitrate yield is slightly higher than the adjusted nitrate yields in the Carter and Atkinson (1996) mechanism because the mechanism generation system included some nitrate formation from peroxy radicals formed in secondary reactions. Although the yields were not readjusted, the mechanism still gives satisfactory fits to the isoprene chamber data used in the nitrate yield adjustments by Carter and Atkinson (1996).

The reactants, products and rate parameter are consistent with current knowledge.

Reaction ISO3

k(300)	A	Ea	Notes	
1.34e-17	7.86e-15	3.80	131, 108, 133, 110	ISOPRENE + O3 = #.066 RO2-R. + #.134 R2O2. + #.266 HO. + #.275 CO + #.122 CO2 + #.6 HCHO + #.1 PROD2 + #.39 METHACRO + #.16 MVK + #.2 MA-RCO3. + #.204 HCOOH + #.15 RCO-OH + #-.251 XC

Notes

131	Isoprene mechanism used is based on the "four product" condensed isoprene mechanism of Carter (1996) which in turn is based on the detailed isoprene mechanism of Carter and Atkinson (1996). The rate constants and the major initial reaction pathways are the same as used in those mechanisms. Some minor changes in product yields resulted in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction schemes, or as indicated in other footnotes.
108	The excited HCHO2 biradical is assumed to react as recommended by Atkinson (1997) based on data for the O3 + ethene system, i.e., 37% stabilization, 12% decomposition to HCO + OH, 13% decomposition to CO2 + H2, and 38% decomposition to CO + H2O. Note that this is different than used for this species when formed in the isoprene products mechanisms of Carter and Atkinson (1996) and Carter (1996).
133	The excited CH2=CHC(O2)CH3 and CH2=C(CH3)CHO2. biradical reactions are the same as given by Carter and Atkinson (1996), except that the CH2=CHC(O)O2. formed from the former is represented by MA-RCO3, and the propene formed from the latter is represented by PROD2.
110	The organic acid(s) formed in this reaction represent the formation of stabilized Crigiee biradicals, which are assumed to be consumed primarily by reaction with H2O forming the corresponding acid.

The reactants, products and rate parameter are consistent with current knowledge. The reaction of stabilized Crigiee with H2O is highly uncertain.

Reaction ISN3

k(300)	A	Ea	Notes	
6.81e-13	3.03e-12	0.89	131, 134	ISOPRENE + NO3 = #.19 NO2 + #.76 RO2-R. + #.05 RO2-N. + #.19 R2O2. + #.95 ISOPROD + #-.05 XC + #.81 XN

Notes

131	Isoprene mechanism used is based on the "four product" condensed isoprene mechanism of Carter (1996) which in turn is based on the detailed isoprene mechanism of Carter and Atkinson (1996). The rate constants and the major initial reaction pathways are the same as used in those mechanisms. Some minor changes in product yields resulted in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction schemes, or as indicated in other footnotes.
134	All the organic products formed in this reaction are represented by ISOPROD. A small amount of nitrate formation is estimated to occur from the reactions of the substituted peroxy radicals with NO (Carter, 1999a).

The reactants, products and rate parameter are consistent with current knowledge.

Reaction ISOP

k(300)	A	Ea	Notes	
3.60e-11	3.60e-11		131, 135	ISOPRENE + O3P = #.25 RO2-R. + #.25 R2O2. + #.5 HCHO + #.75 PROD2 + #.25 MA-RCO3. + #-1 XC

Notes

131	Isoprene mechanism used is based on the "four product" condensed isoprene mechanism of Carter (1996) which in turn is based on the detailed isoprene mechanism of Carter and Atkinson (1996). The rate constants and the major initial reaction pathways are the same as used in those mechanisms. Some minor changes in product yields resulted in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction schemes, or as indicated in other footnotes.
135	PROD2 is used to represent the various isoprene oxide products. And MA-RCO3 us used to represent CH2=CHC(O)OO. Note that this mechanism, which is based on that of Carter and Atkinson (1996) is inconsistent with the mechanisms for the reactions of O3P with the other higher alkenes, which are assumed not to form radical products. However, assuming no radical formation in the reaction of O3P with isoprene results in somewhat degraded model performance in simulations of the results of the isoprene experiments discussed by Carter and Atkinson (1996).

The reactants, products and rate parameter are estimated and therefore have a high degree of uncertainty. The reaction is probably not important in air under most conditions.